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Fundamental optimal relation of a spin 1/2 quantum Brayton heat engine with multi-irreversibilities

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Abstract In this paper, an irreversible quantum Brayton heat engine cycle model composed of two isomagnetic processes and two irreversible adiabatic processes is established. The quantum heat engine works with non-interacting spin-1/2 systems and has multi-irreversibilities. By using detailed numerical examples, this paper gives the fundamental optimal relationship of the quantum Brayton heat engine, in a general case and at high temperature limits, and analyzes the effects of internal friction and bypass heat leakage on the fundamental optimal relationship. Comparisons of the power output versus efficiency characteristics among this spin quantum heat Brayton engine, a quantum spin Carnot heat engine and a Brayton heat engine working with a classical working medium, are made. Three special cases, such as the endoreversible case, the frictionless case and the case without bypass heat leakage, are discussed.

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1. Introduction

Performance analyses of heat engines have been a major source of thermodynamic insight, and have led to a connection between abstract thermodynamic theories and realizable physical phenomena. Finite Time Thermodynamics (FTT), which began from the study of the Newtonian law endoreversible Carnot engine system [1], have made considerable progress [2–8]. However, for some special fields and systems, such as the quantum amplifier, laser cooling, aerospace, superconductivity applications, infra-red techniques and so on, the working medium of these systems obeys the law of quantum statistical mechanics, and the quantum characteristic of the working medium has to be considered in the performance investigation of these systems. In recent years, many authors have extended the objectives of FTT to quantum thermodynamic systems, such as

quantum heat engines, refrigerators and heat pumps, by combining the semi-group approach and quantum master equation, and have obtained many meaningful results.

In the performance analysis and optimization of quantum thermodynamic systems, the working medium are several typical quantum mechanical systems, such as non-interacting harmonic oscillators [9–12] and spin-1/2 systems [13–16], ideal quantum gas [17–20] and microscope particles confined to a potential well [21]. Besides the quantum Carnot cycle, quantum thermodynamic cycles may be the Brayton cycle, the Ericsson cycle [14,15,22], the Otto cycle [20], the Stirling cycle [23–26], and so on. Similar to thermodynamic systems with a classical working medium, the endoreversible cycles are the basic models, otherwise some authors have established irreversible models by considering the irreversibility of internal irreversibility [27,28], bypass heat leakage [29] and inherent regeneration [12,22,30]. Some authors have established general irreversible models [15,31,32] by considering the irreversibilities of heat resistance, internal irreversibility (described by an internal irreversible factor) and bypass heat leakage, and general irreversible heat engine models [33], considering the irreversibilities of heat resistance, internal friction (described by an internal friction coefficient) and bypass heat leakage.

A Brayton heat engine cycle with a classical working medium consists of two adiabatic and two constant-pressure branches, and a quantum Brayton heat engine cycle with spin systems

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Nomenclature

a	Parameter of heat reservoir (s^{-1})
B	Heat reservoir
$\vec{B}$	External magnetic field (T)
C_e	Dimensionless factor that describes the magnitude of the bypass heat leakage
c	Parameter of heat reservoir (s^{-1})
E_S	Internal energy of the spin-1/2 systems (J)
$\hat{H}$	Hamiltonian
$\hbar$	Reduced Planck's constant ($J \cdot s$)
k_B	Boltzmann constant (J/K)
L_1, L_2, L_3, L_4	Lagrangian functions
$\hat{M}$	Magnetic moment operator
n_c	Population of the thermal phonons of the cold reservoir
P	Power output (W)
Q	Amount of heat exchange (J)
$\hat{Q}_\alpha, \hat{Q}_\alpha^+$	Operator in the Hilbert space of the system and Hermitian conjugates
$\dot{Q}_e$	Rate of heat flow of bypass heat leakage (W)
q	Parameter of heat reservoir
S	Expectation value of spin operator $\hat{S}_z$
$\hat{S}_+, \hat{S}_-$	Spin creation and annihilation operators
$\hat{S}(\hat{S}_x, \hat{S}_y, \hat{S}_z)$	Spin operator
S_{eq}	Asymptotic value of S
T	Absolute temperature (K)
t	Time (s)
W	Work (J)

Greek symbols

α	Intermediate variable
β	Temperature, $\beta = 1/(k_B T)$ (J^{-1})
γ_+, γ_-	Phenomenological positive coefficients
η	Efficiency
λ	Parameter of the heat reservoir
$\lambda_1, \lambda_2, \lambda_3, \lambda_4$	Lagrangian multipliers
μ	Friction coefficient
μ_B	Bohr magneton (J/T)
$\hat{F}$	Interaction strength operator
τ	Time (s)/cycle period (s)
ω	The magnetic field, $\omega = 2 \mu_B B(t)_z$

Subscripts

B	Heat reservoir
c	Cold side
h	Hot side
S	Working medium system
SB	Interaction between heat reservoir and working medium system
$\max, \mu = 0, C_e = 0$	Maximum point for endoreversible case
1, 2, 3, 4	Cycle states

consists of two adiabatic and two isomagnetic field branches. In the investigation of quantum Brayton cycles, Feldmann et al. [34] were the first to establish an endoreversible quantum Brayton heat engine model, working with non-interacting spin systems, and investigated its optimal performance. Lin and Chen [35] established an endoreversible quantum Brayton

heat engine model working with non-interacting harmonic oscillators, and investigated its optimal performance. Feldmann and Kosloff [36] introduced an internal friction, and established an irreversible quantum spin Brayton heat engine and heat pump models. The internal friction describes the quantum non-adiabatic phenomenon caused by rapid change in the external magnetic field in the adiabatic process, which has an obvious effect on the performance of the quantum heat engine and heat pump. Since then, the origin and effects of quantum friction on the performance of quantum thermodynamic cycles have become interesting research subjects [33,37–41]. By taking into account heat resistance, internal irreversibility and bypass heat leakage, Wu et al. [32] established a generalized irreversible harmonic quantum Brayton heat engine model, and investigated the optimal performance of the two quantum heat engines.

Unlike the previous study [32], this paper will establish a generalized irreversible quantum Brayton heat engine model working with non-interacting spin systems. The irreversibilities of heat resistance, internal friction in the adiabatic processes, and bypass heat leakage are taken into account in this model. This paper will derive the cycle period, power output and efficiency by using FTT, the semi-group approach and a quantum master equation. By using detailed numerical examples and illustrations, this paper will give the fundamental optimal relationship of the quantum Brayton heat engine and analyze the effects of internal friction and bypass heat leakage on the fundamental optimal relationship. At high temperature limits, the performance parameters of the quantum Brayton heat engine will be simplified, and the fundamental optimal relationship will also be obtained using detailed numerical examples. Comparisons of the power output versus efficiency characteristics between this quantum spin heat Brayton engine, a Brayton heat engine working with classical working medium, and a quantum spin Carnot heat engine, will be made. Three special cases (endoreversible, frictionless and without bypass heat leakage) will be discussed in brief. The results obtained are general and can enrich the FTT theory for quantum thermodynamic cycles.

2. Quantum dynamics of a spin-1/2 system

In this section, one considers a single spin-1/2 particle placed in a time dependent magnetic field, $\vec{B}$, and the direction of the magnetic field is along the positive z axis. The Hamiltonian of the interaction between a magnetic moment, $\hat{M}$, and the magnetic field, $\vec{B}$, is $\hat{H}(t) = -\hat{M} \cdot \vec{B}$. For a single spin-1/2 system, the Hamiltonian is given by Zeng [42]:

$$\hat{H}_S = -\hat{M} \cdot \vec{B} = 2 \mu_B \hat{S} \cdot \vec{B} / \hbar = 2 \mu_B \hat{S}_z B_z / \hbar = \omega(t) \hat{S}_z / \hbar, \quad (1)$$

where $\hat{S}$ is a spin angular momentum, which is along the positive $\hat{M}$ directions, μ_B is the Bohr magnetron, $\hbar$ is the reduced Planck's constant and $\omega(t) = 2 \mu_B B(t)_z$. One refers to ω rather than B_z as “the magnetic field” throughout this paper. The internal energy of the spin system is given by:

$$E_S = \langle \hat{H}_S \rangle = \omega \langle \hat{S}_z \rangle / \hbar = \omega S / \hbar, \quad (2)$$

where:

$$S = \langle \hat{S}_z \rangle = -\frac{\hbar}{2} \tanh \left(\frac{\beta \omega}{2} \right), \quad (3)$$

is the expectation value of $\hat{S}_z$, $\beta = 1/(k_B T)$, k_B is the Boltzmann constant and T is the absolute temperature. For simplicity, one refers to β rather than T as the “temperature” throughout this paper.

For a spin-1/2 system coupled thermally to a heat reservoir (bath), the system-bath Hamiltonian is given by:

$$\hat{H} = \hat{H}_S + \hat{H}_{SB} + \hat{H}_B, \quad (4)$$

where $\hat{H}_S$, $\hat{H}_{SB}$ and $\hat{H}_B$ are, respectively, Hamiltonians of the spin-1/2 system, the system-bath and the bath. In the Heisenberg picture, the motion of an operator of the spin-1/2 system is given by the quantum master equation:

$$\frac{d\hat{X}}{dt} = \frac{i}{\hbar} [\hat{H}_S, \hat{X}] + \frac{\partial \hat{X}}{\partial t} + L_D(\hat{X}), \quad (5)$$

where $L_D(\hat{X})$ is a dissipation term (the relaxation-type term includes the effects of $\hat{H}_{SB}$ and $\hat{H}_B$), which originates from a thermal system-bath coupling. Using a semi-group approach, one gives the dissipation term [43,44]:

$$L_D(\hat{X}) = \sum_{\alpha} \gamma_{\alpha} (\hat{Q}_{\alpha}^+ [\hat{X}, \hat{Q}_{\alpha}] + [\hat{Q}_{\alpha}^+, \hat{X}] \hat{Q}_{\alpha}), \quad (6)$$

where γ_{α} are phenomenological positive coefficients, and $\hat{Q}_{\alpha}$ and $\hat{Q}_{\alpha}^+$ are system operators in Hilbert space, which are Hermitian conjugates.

Substituting the system Hamiltonian, $\hat{X} = \hat{H}_S$, into Eq. (5), gives the internal energy change rate:

$$\begin{aligned} \frac{dE_S}{dt} &= \frac{d}{dt} \langle \hat{H}_S \rangle = \left\langle \frac{\partial \hat{H}_S}{\partial t} \right\rangle + \langle L_D(\hat{H}_S) \rangle \\ &= S \frac{d\omega}{dt} / \hbar + \omega \frac{dS}{dt} / \hbar. \end{aligned} \quad (7)$$

Comparing Eq. (7) with the differential form of the first law of thermodynamics:

$$\frac{dE_S}{dt} = \frac{dW}{dt} + \frac{dQ}{dt}. \quad (8)$$

One can find that the instantaneous heat flow and power may be identified by:

$$\dot{Q} = \langle L_D(\hat{H}_S) \rangle = \omega \dot{S} / \hbar = dQ/dt, \quad (9)$$

$$P = \langle \partial \hat{H}_S / \partial t \rangle = \dot{\omega} S / \hbar = dW/dt. \quad (10)$$

Hence, heat and work inexact differentials are given by:

$$dQ = \omega dS / \hbar, \quad (11)$$

$$dW = S d\omega / \hbar. \quad (12)$$

For a spin-1/2 system, Eq. (7) gives the time derivative form of the first law of thermodynamics.

In order to obtain the change rate of spin angular momentum S when the spin-1/2 system couples with a heat bath, one chooses $\hat{Q}_{\alpha}^+ = \hat{S}_+ = \hat{S}_x + i\hat{S}_y$ and $\hat{Q}_{\alpha} = \hat{S}_- = \hat{S}_x - i\hat{S}_y$ in Eq. (6). Substituting $\hat{Q}_{\alpha}^+$ and $\hat{Q}_{\alpha}$ into Eq. (5) and using the commutation relations, $[\hat{S}_x, \hat{S}_y] = i\hbar \hat{S}_z$, $[\hat{S}_y, \hat{S}_z] = i\hbar \hat{S}_x$, $[\hat{S}_z, \hat{S}_x] = i\hbar \hat{S}_y$ and $\hat{S}_x^2 = \hat{S}_y^2 = \hat{S}_z^2 = \frac{\hbar^2}{4}$ gives:

$$\dot{S} = -2\hbar^2(\gamma_+ + \gamma_-)S - \hbar^3(\gamma_- - \gamma_+). \quad (13)$$

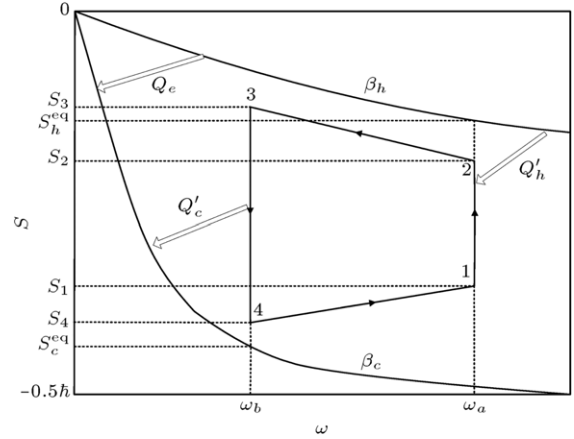


Figure 1: The $S - \omega$ diagram of an irreversible quantum spin Brayton heat engine with multi-irreversibilities.

If the field, ω , is constant, coefficients, γ_+ and γ_- , are both constants. Solving Eq. (13) gives:

$$S(t) = S_{eq} + [S(0) - S_{eq}]e^{-(\gamma_+ + \gamma_-)t}, \quad (14)$$

where $S(0)$ is the initial spin angular momentum, $S_{eq} = -\hbar(\gamma_- - \gamma_+)/2(\gamma_- + \gamma_+)$ is the asymptotic spin angular momentum, which must correspond to the equilibrium spin angular momentum, $S_{eq} = -\frac{\hbar}{2} \tanh(\frac{\beta_j \omega}{2})$, where β_j is the temperature of the heat bath. Comparing the two expressions of S_{eq} gives $\gamma_-/\gamma_+ = e^{\beta_j \omega}$, so that one assumes simply that:

$$\gamma_+ = ae^{q\beta_j \omega}, \quad (15)$$

$$\gamma_- = ae^{(1+q)\beta_j \omega}, \quad (16)$$

where a and q are two constants. At the weak-coupling limit, the explicit expressions of γ_+ and γ_- can be obtained in terms of correlation functions of the bath [45]. γ_+ , $\gamma_- > 0$ requires $a > 0$. If $\beta_j \omega \rightarrow \infty$, $\gamma_+ \rightarrow 0$ and $\gamma_- \rightarrow \infty$ hold, it requires $0 > q > -1$. Substituting Eqs. (15) and (16) into Eq. (13) yields the change rate of the spin angular momentum:

$$\dot{S} = -a\hbar^2 e^{q\beta \omega} [2(1 + e^{\beta \omega})S + \hbar(e^{\beta \omega} - 1)]. \quad (17)$$

3. An irreversible spin quantum Brayton heat engine model

(1) The quantum heat engine uses many non-interacting spin-1/2 systems as a working medium. The spin-1/2 system in the engine couples mechanically to a time dependent external “magnetic field” and is a two level system. The direction of the external magnetic field is along the positive z axis. The magnitude of the field is not allowed to reach zero, where the two energy levels of the spin system are degenerate.

(2) The quantum heat engine operates between a hot reservoir, B_h , and a cold reservoir, B_c . The two reservoirs are thermal phonon systems and are at constant temperature, β_h at β_c , respectively. One assumes that the heat reservoirs are infinitely large and their internal relaxations are very strong, so that they can be assumed to be in thermal equilibrium.

(3) The quantum Brayton heat engine cycle is composed of two isomagnetic branches (process $1 \rightarrow 2$ with $\omega = \omega_a$ and process $3 \rightarrow 4$ with $\omega = \omega_b$) connected by two irreversible adiabatic branches (processes $2 \rightarrow 3$ and $4 \rightarrow 1$), and the $S - \omega$ diagram of the cycle is shown in Figure 1.

In the two isomagnetic processes, the working medium couples to the heat reservoirs for a finite time, τ_h and τ_c ,

respectively, and exchange heat, Q_{12} and Q_{34} , with the heat reservoirs. The finite rate of the heat transfer requires $\beta_c > \beta_4 > \beta_1 > \beta_2 > \beta_h$ where β_1, β_2 and β_4 are the temperatures of the working medium in states 1, 2 and 4, respectively. Using Eq. (11), one can calculate the amounts of heat the working medium absorbs from the hot reservoir in isomagnetic process $1 \rightarrow 2$:

$$Q_{12} = \frac{1}{\hbar} \int_1^2 \omega dS = \frac{1}{\hbar} \omega_a (S_2 - S_1) = \frac{\omega_a}{2} \left[\tanh\left(\frac{\beta_1 \omega_a}{2}\right) - \tanh\left(\frac{\beta_2 \omega_a}{2}\right) \right]. \quad (18)$$

From Eq. (12), one finds that there is no work done by the working medium along the isomagnetic processes because of constant ω .

In the adiabatic processes $2 \rightarrow 3$ and $4 \rightarrow 1$, there is no thermal coupling between the working medium and the heat reservoirs, so there is no heat exchange. In the adiabatic process $2 \rightarrow 3$ (or $4 \rightarrow 1$), the external magnetic field varies linearly in time from ω_a (or ω_b) to ω_b (or ω_a) in a period of τ_a (or τ_b), viz:

$$\omega(t) = \omega(0) + \dot{\omega}t. \quad (19)$$

According to the quantum adiabatic theorem [42], rapid change, $\dot{\omega}$, of the field causes a quantum non-adiabatic phenomenon, which causes an increase in spin angular momentum, S . From Eq. (11), one understands that an increase in S means heat generation, i.e. work dissipation in the adiabatic process. One assumes that there exists a friction coefficient, μ , to describe the non-adiabatic phenomenon [36]:

$$\dot{S} = \hbar \left(\frac{\mu}{t'} \right)^2, \quad (20)$$

where t' is the time of the adiabatic process. The spin angular momentum is given by:

$$S(t) = S(0) + \hbar \left(\frac{\mu}{t'} \right)^2 t, \quad (21)$$

where $0 \leq t \leq t'$. Substituting $t' = \tau_a$ and $t' = \tau_b$, respectively, into Eq. (21) yields:

$$S_2 = S(\tau_a) = S_1 - \hbar \mu^2 / \tau_a, \quad (22)$$

$$S_4 = S(\tau_b) = S_1 - \hbar \mu^2 / \tau_b, \quad (23)$$

where $S_1 = -\frac{\hbar}{2} \tanh \frac{\beta_1 \omega_a}{2}$ and $S_3 = -\frac{\hbar}{2} \tanh \frac{\beta_3 \omega_b}{2}$ are the spin angular momentums at states 1 and 3, respectively. From Eqs. (3), (22) and (23), one can obtain the temperatures of the working medium at states 2 and 4, respectively:

$$\beta_2 = \frac{2}{\omega_a} \tanh^{-1} \left(\tanh \frac{\beta_3 \omega_b}{2} + \frac{2\mu^2}{\tau_a} \right), \quad (24)$$

$$\beta_4 = \frac{2}{\omega_b} \tanh^{-1} \left(\tanh \frac{\beta_1 \omega_a}{2} + \frac{2\mu^2}{\tau_b} \right). \quad (25)$$

From Eqs. (3), (24) and (25), one can obtain the upper bound of β_1 and the lower bound of β_3 :

$$\beta_1 < \beta_{1r} = \frac{2}{\omega_a} \tanh^{-1} \left(\tanh \frac{\beta_c \omega_b}{2} - \frac{2\mu^2}{\tau_b} \right), \quad (26)$$

$$\beta_3 > \beta_{3r} = \frac{2}{\omega_b} \tanh^{-1} \left(\tanh \frac{\beta_h \omega_a}{2} - \frac{2\mu^2}{\tau_a} \right). \quad (27)$$

The work done by the working medium along the adiabatic processes is equal to the internal energy changes, due to the fact that there is no heat exchange between the working medium and heat reservoirs. Using Eqs. (7), (19) and (21), one can obtain:

$$W_{23} = - \int_0^{\tau_a} dE_S = - \frac{1}{\hbar} \int_0^{\tau_a} S d\omega - \frac{1}{\hbar} \int_0^{\tau_a} \omega dS = (\omega_a - \omega_b) \left(\frac{S_3}{\hbar} - \frac{\mu^2}{2\tau_a} \right) - \frac{\mu^2(\omega_a + \omega_b)}{2\tau_a}, \quad (28)$$

$$W_{41} = - \int_0^{\tau_b} dE_S = - \frac{1}{\hbar} \int_0^{\tau_b} S d\omega - \frac{1}{\hbar} \int_0^{\tau_b} \omega dS = (\omega_b - \omega_a) \left(\frac{S_1}{\hbar} - \frac{\mu^2}{2\tau_b} \right) - \frac{\mu^2(\omega_a + \omega_b)}{2\tau_b}. \quad (29)$$

The second parts of W_{23} and W_{41} , i.e. $\frac{\mu^2(\omega_a + \omega_b)}{2\tau_a}$ and $\frac{\mu^2(\omega_a + \omega_b)}{2\tau_b}$, is the work done against the internal friction along the adiabatic processes, $2 \rightarrow 3$ and $4 \rightarrow 1$, respectively.

(4) The quantum Brayton heat engine has a bypass heat leakage between hot and cold reservoirs. It arises from the thermal coupling action between the hot and cold reservoirs by the working medium.

As mentioned above, the hot and cold reservoirs are both thermal phonon systems, B_h and B_c , respectively. One assumes that the creation and annihilation operators of the phonons in the hot and cold reservoirs are, respectively, $\hat{b}_h^+$, $\hat{b}_h^-$, $\hat{b}_c^+$ and $\hat{b}_c^-$, and the phonon frequency and population of the cold reservoir are, respectively, $\omega_c(t)$ and $n_c = 1/(e^{\hbar\omega_c\beta_c} - 1)$. When there exists a thermal coupling action between the hot and cold reservoirs by the working medium, the heat reservoirs become an open system. Similar to the derivation of $\dot{S}$ in Section 2, one can derive the time derivative of the population of the cold heat reservoir, n_c , by solving the quantum master equation of the heat reservoirs [29]:

$$\dot{n}_c = -2C_e \lambda \hbar \beta_h \omega_c [(e^{\hbar\beta_h \omega_c} - 1)n_c - 1], \quad (30)$$

where c and λ are constants. By using the instantaneous heat flow definition for the harmonic oscillators system, $\dot{Q} = \omega \dot{n}$ [10], the rate of bypass heat leakage (rate of heat flow from the hot reservoir to the cold reservoir) is given by:

$$\dot{Q}_e = C_e \hbar \omega_c \dot{n}_c = 2C_e c \hbar \omega_c e^{\lambda \hbar \beta_h \omega_c} [1 - (e^{\hbar\beta_h \omega_c} - 1)n_c], \quad (31)$$

where C_e is a dimensionless factor one introduces to describe the magnitude of the bypass heat leakage. One assumes that $\dot{Q}_e$ is a constant, therefore, the bypass heat leakage quantity, Q_e , per cycle, is given by:

$$Q_e = \dot{Q}_e \tau = 2C_e c \hbar \omega_c e^{\lambda \hbar \beta_h \omega_c} [1 - (e^{\hbar\beta_h \omega_c} - 1)n_c] \tau. \quad (32)$$

The model studied in this paper is similar to the model of classical generalized irreversible simple Brayton heat engines with multi-irreversibilities, such as heat resistance, internal irreversibility and bypass heat leakage [46–51].

4. Cycle period

From Eq. (17), one can calculate the time of isomagnetic processes $1 \rightarrow 2$ and $3 \rightarrow 4$, respectively:

$$\tau_h = \int_{S_1}^{S_2} \frac{dS}{\dot{S}} = \frac{1}{2a \hbar^2 e^{a\beta_h \omega_a} (e^{\beta_h \omega_a} + 1)} \times \ln \left[\frac{\tanh(\beta_h \omega_a/2) - \tanh(\beta_1 \omega_a/2)}{\tanh(\beta_h \omega_a/2) - \tanh(\beta_3 \omega_b/2) - 2\mu^2/\tau_a} \right], \quad (33)$$

$$\tau_c = \int_{S_3}^{S_4} \frac{dS}{\dot{S}} = \frac{1}{2a\hbar^2 e^{q\beta_c\omega_b} (e^{\beta_c\omega_b} + 1)} \times \ln \left[\frac{\tanh(\beta_c\omega_b/2) - \tanh(\beta_3\omega_b/2)}{\tanh(\beta_c\omega_b/2) - \tanh(\beta_1\omega_a/2) - 2\mu^2/\tau_b} \right]. \quad (34)$$

The cycle period is given by:

$$\tau = \tau_h + \tau_c + \tau_a + \tau_b. \quad (35)$$

5. Fundamental optimal relationship

Using Eqs. (28) and (29) yields the total work output per cycle of the quantum Brayton heat engine:

$$\begin{aligned} W &= \oint dW = W_{12} + W_{23} + W_{34} + W_{41} \\ &= \frac{1}{2}(\omega_a - \omega_b) \left[\tanh\left(\frac{\beta_1\omega_a}{2}\right) - \tanh\left(\frac{\beta_3\omega_b}{2}\right) \right] \\ &\quad - \mu^2 \left(\frac{\omega_a}{\tau_a} + \frac{\omega_b}{\tau_b} \right). \end{aligned} \quad (36)$$

Using Eq. (35) with Eq. (36) yields the power output of the quantum heat engine:

$$\begin{aligned} P = \frac{W}{\tau} &= \left\{ \frac{1}{2}(\omega_a - \omega_b) \left[\tanh\left(\frac{\beta_1\omega_a}{2}\right) - \tanh\left(\frac{\beta_3\omega_b}{2}\right) \right] \right. \\ &\quad \left. - \mu^2 \left(\frac{\omega_a}{\tau_a} + \frac{\omega_b}{\tau_b} \right) \right\} \tau^{-1}. \end{aligned} \quad (37)$$

Using Eqs. (18), (32) and (36) yields the efficiency of the quantum heat engine: Eq. (38) is given in Box I, where $Q_h = Q_{12} + Q_e$ is the total heat released by the hot reservoir per cycle.

Using numerical calculation, one can plot three-dimensional diagrams of the power output ($P/P_{\max, \mu=0, C_e=0}$, β_1, β_3) and efficiency (η, β_1, β_3) from Eqs. (37) and (38) where $P_{\max, \mu=0, C_e=0}$ is the maximum power output for the endoreversible case ($\mu = 0, C_e = 0$), as shown in Figures 2 and 3. According to Refs. [34,36], $\hbar = 1$ and $k_B = 1$ are set in the numerical calculations for simplicity. The parameters used in the numerical calculations are $a = c = 2, q = \lambda = -0.5, \beta_h = 0.2, \beta_c = 1, \tau_a = \tau_b = 0.01, \omega_1 = 5, \omega_3 = 3, \omega_c = 0.2, \mu = 0.002$ and $C_e = 0.05$. From Figure 2, one can see that there exist optimal temperatures, β_1 and β_3 , which lead to the maximum power output of the quantum Brayton heat engine. Affected by the internal friction and bypass heat leakage, the maximum dimensionless power output $(P/P_{\max, \mu=0, C_e=0})_{\max} < 1$. Figure 3 shows that there also exist optimal temperatures, β_1 and β_3 , which lead to maximum efficiency when there exists a bypass heat leakage.

For the quantum Brayton heat engine, to determine the maximum power output for fixed efficiency or maximum efficiency for a fixed power output, one introduces Lagrangian functions; $L_1 = P + \lambda_1 \eta$ and $L_2 = \eta + \lambda_2 P$, where λ_1 and λ_2 are two Lagrangian multipliers. Theoretically, by combining Eqs. (37) and (38) and the extreme conditions, one can obtain the optimal relation between β_1 and β_3 , and then obtain the fundamental optimal relationship. The extreme conditions are given by the Euler-Lagrange equation:

$$\partial L_1 / \partial \beta_1 = 0, \quad \partial L_1 / \partial \beta_3 = 0, \quad (39)$$

or:

$$\partial L_2 / \partial \beta_1 = 0, \quad \partial L_2 / \partial \beta_3 = 0, \quad (40)$$

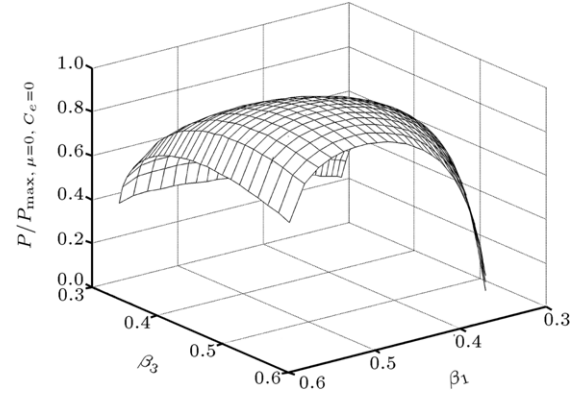


Figure 2: The dimensionless power output $P/P_{\max, \mu=0, C_e=0}$ versus “temperatures” β_1 and β_3 .

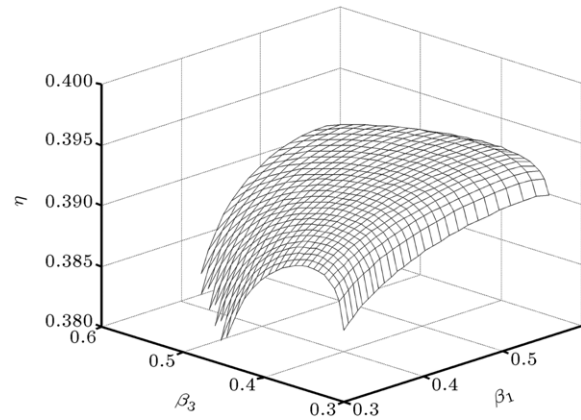


Figure 3: The efficiency η versus “temperatures” β_1 and β_3 .

However, because of the strong complexity and nonlinearity of these equations, one cannot solve these equations analytically, and obtain fundamental optimal relations analytically. With the same parameters used in the calculation of Figure 2, one can plot the dimensionless power output versus efficiency characteristic curves, $P/P_{\max, \mu=0, C_e=0} - \eta$, by solving the Euler-Lagrange

Eq. (39) or (40), numerically, as shown in Figure 4. One can see from Figure 4 that the efficiency is a constant (for given ω_b/ω_a) when there exists no internal friction and bypass heat leakage. When a bypass heat leakage exists, the $P/P_{\max, \mu=0, C_e=0} - \eta$ curve is monotonic increasing. When internal friction exists, the $P/P_{\max, \mu=0, C_e=0} - \eta$ curve is parabolic-like. When both internal friction and bypass heat leakage exists, the $P/P_{\max, \mu=0, C_e=0} - \eta$ curve becomes loop-shaped. The internal friction decreases both power output and efficiency, while the bypass heat leakage only decreases efficiency.

6. Fundamental optimal relationship at high temperature limit

When the temperatures of heat reservoirs and the working medium are high enough, i.e. $\beta\omega \ll 1$, the results obtained above can be simplified. For example, Eqs. (3), (31) and (33)–(38) can be simplified at the first order approximation: Eqs. (41)–(48) are given in Box II where:

$$\alpha = \frac{2c\hbar\omega_c(1 + \lambda\hbar\beta_h\omega_c)}{\beta_c}.$$

$$\eta = \frac{W}{Q_h} = \frac{(\omega_a - \omega_b) \left[\tanh\left(\frac{\beta_1 \omega_a}{2}\right) - \tanh\left(\frac{\beta_3 \omega_b}{2}\right) \right] - 2\mu^2 \left(\frac{\omega_a}{\tau_a} + \frac{\omega_b}{\tau_b} \right)}{\omega_a \left[\tanh\left(\frac{\beta_1 \omega_a}{2}\right) - \tanh\left(\frac{\beta_3 \omega_b}{2}\right) - \frac{2\mu^2}{\tau_a} \right] + 4C_e \hbar \omega_c e^{\lambda \hbar \beta_h \omega_c} [1 - (e^{\hbar \beta_h \omega_c} - 1)n_c] \tau} \quad (38)$$

Box I:

$$S = -\frac{\hbar}{4}\beta\omega, \quad (41)$$

$$\dot{Q}_e \approx C_e \frac{2\hbar\omega_c(1 + \lambda\hbar\beta_h\omega_c)}{\beta_c} (\beta_c - \beta_h) = C_e \alpha (\beta_c - \beta_h), \quad (42)$$

$$\tau_h = \frac{1}{4a\hbar^2} \ln \left[\frac{\tau_a \omega_a (\beta_h - \beta_1)}{\tau_a \omega_a \beta_h - \beta_3 \omega_b \tau_a - 4\mu^2} \right], \quad (43)$$

$$\tau_c = \frac{1}{4a\hbar^2} \ln \left[\frac{\tau_b \omega_b (\beta_c - \beta_3)}{\tau_b \omega_b \beta_c - \beta_1 \omega_a \tau_b - 4\mu^2} \right], \quad (44)$$

$$\tau = \frac{1}{4a\hbar^2} \ln \frac{\omega_a \omega_b \tau_a \tau_b (\beta_h - \beta_1)(\beta_c - \beta_3)}{(\tau_a \omega_a \beta_h - \beta_3 \omega_b \tau_a - 4\mu^2)(\tau_b \omega_b \beta_c - \beta_1 \omega_a \tau_b - 4\mu^2)} + \tau_a + \tau_b, \quad (45)$$

$$W = \frac{(\omega_a - \omega_b)(\beta_1 \omega_a - \beta_3 \omega_b)}{4} - \mu^2 \left(\frac{\omega_a}{\tau_a} + \frac{\omega_b}{\tau_b} \right), \quad (46)$$

$$P = \frac{a\hbar^2(\omega_a - \omega_b)(\beta_1 \omega_a - \beta_3 \omega_b) - 4a\hbar^2\mu^2(\tau_a \omega_b + \tau_b \omega_a)}{\tau_a \tau_b \ln \frac{\omega_a \omega_b \tau_a \tau_b (\beta_h - \beta_1)(\beta_c - \beta_3)}{(\tau_a \omega_a \beta_h - \beta_3 \omega_b \tau_a - 4\mu^2)(\tau_b \omega_b \beta_c - \beta_1 \omega_a \tau_b - 4\mu^2)} + 4a\hbar^2\tau_a \tau_b (\tau_a + \tau_b)}, \quad (47)$$

$$\eta = \frac{a\hbar^2\tau_a \tau_b (\omega_a - \omega_b)(\beta_1 \omega_a - \beta_3 \omega_b) - 4a\hbar^2\mu^2(\tau_a \omega_b + \tau_b \omega_a)}{\left\{ a\hbar^2\omega_a \tau_b (\tau_a \omega_a \beta_1 - \beta_3 \tau_a \omega_b - 4\mu^2) + \tau_a \tau_b C_e \alpha (\beta_c - \beta_h) \right.} \\ \left. \times \left[\ln \frac{\omega_a \omega_b \tau_a \tau_b (\beta_h - \beta_1)(\beta_c - \beta_3)}{(\tau_a \omega_a \beta_h - \beta_3 \omega_b \tau_a - 4\mu^2)(\tau_b \omega_b \beta_c - \beta_1 \omega_a \tau_b - 4\mu^2)} + 4a\hbar^2(\tau_a + \tau_b) \right] \right\} \quad (48)$$

Box II:

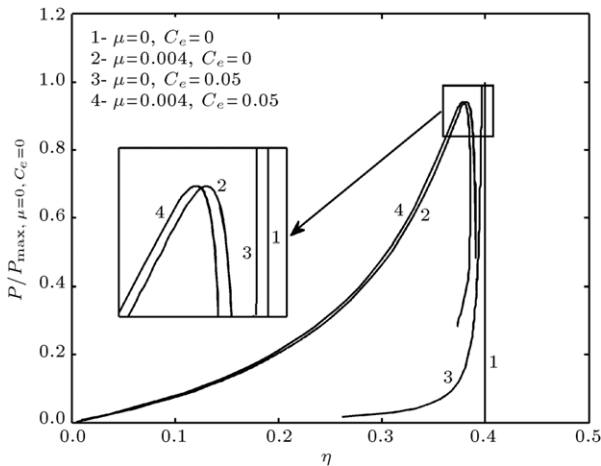


Figure 4: The effects of μ and C_e on dimensionless power output $P/P_{\max, \mu=0, C_e=0}$ versus efficiency η .

Similar to Figures 2 and 3, one can plot three-dimensional diagrams of the power output ($P/P_{\max, \mu=0, C_e=0}$, β_1 , β_3) and efficiency (η , β_1 , β_3) from Eqs. (47) and (48), where $P_{\max, \mu=0, C_e=0}$ is the maximum power output for an endoreversible case ($\mu = 0$, $C_e = 0$) at high temperature limits. For simplicity, these two, three-dimensional diagrams are not given here. At high temperature limits, one can see that the relationship between dimensionless power output (or efficiency) and temperatures, β_1 and β_3 , is similar to that of a general case. The dimensionless power

output has a maximum, and when bypass heat leakage exists, the efficiency has a maximum that has a nonzero corresponding power output.

For the quantum Brayton heat engine, to determine the maximum power output for fixed or maximum efficiency for a fixed power output, one introduces Lagrangian functions, $L_3 = P + \lambda_3 \eta$ and $L_4 = \eta + \lambda_4 P$ where λ_3 and λ_4 are two Lagrangian multipliers. The Euler-Lagrange equations become:

$$\partial L_3 / \partial \beta_1 = 0, \quad \partial L_3 / \partial \beta_3 = 0, \quad (49)$$

or:

$$\partial L_4 / \partial \beta_1 = 0, \quad \partial L_4 / \partial \beta_3 = 0. \quad (50)$$

With the help of Eqs. (47) and (48), one can solve Eq. (49) or (50), numerically, and obtain the fundamental optimal relationship of the quantum Brayton heat engine at high temperature limit, as shown in Figure 5. According to Refs. [34,36], the parameter values used in the numerical calculations are:

$$a = c = 2, \quad q = \lambda = -0.5, \quad \beta_h = 0.001, \\ \beta_c = 1/290, \quad \tau_a = \tau_b = 0.01, \quad \omega_1 = 10, \\ \omega_3 = 8, \quad \omega_c = 6.$$

From Figure 5, one can see that the efficiency, η , is constant (for given ω_b/ω_a) and the $P/P_{\max, \mu=0, C_e=0} - \eta$ curve is a beeline when no internal friction and bypass heat leakage exist. The internal friction makes the $P/P_{\max, \mu=0, C_e=0} - \eta$ curve become parabolic-like, while the bypass heat leakage makes the $P/P_{\max, \mu=0, C_e=0} - \eta$ curve become monotonic increasing.

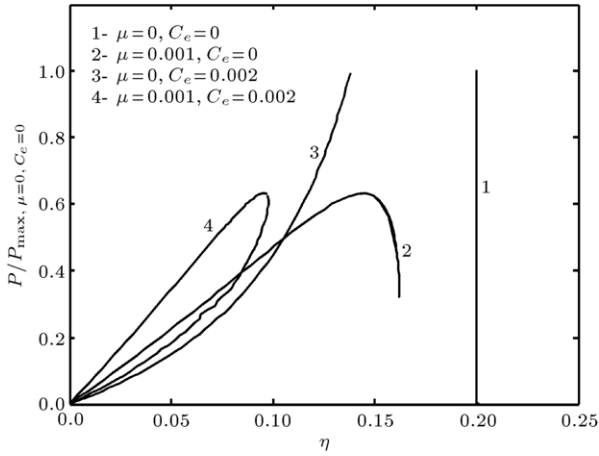


Figure 5: The Effects of μ and C_e on dimensionless power output $P/P_{\max, \mu=0, C_e=0}$ versus efficiency η at high temperature limit.

When both internal friction and bypass heat leakage exist, the $P/P_{\max, \mu=0, C_e=0} - \eta$ curve becomes loop-shaped.

The fundamental optimal relationship of the irreversible spin quantum Brayton heat engine is different to those of an irreversible spin quantum Carnot heat engine [31] and an irreversible Brayton heat engine with classical working medium [51]. The $P/P_{\max, \mu=0, C_e=0} - \eta$ curves of the spin quantum Carnot heat engine and the Brayton heat engine with classical working medium are both parabolic-like for an endoreversible case, and the bypass heat leakage changes the $P/P_{\max, \mu=0, C_e=0} - \eta$ curves to loop-shaped. The internal irreversibility only affects the power output versus efficiency characteristic, quantitatively. The difference means that the quantum characteristic of the working medium does affect the performance of the quantum heat engine, and it is necessary for one to consider the quantum characteristic of the working medium in the performance investigation of a quantum heat engine.

7. Three special cases

The results obtained above include the fundamental optimal relations in an endoreversible case, a frictionless case and a case without bypass heat leakage.

Case 1: Endoreversible case (i.e. $\mu = 0$ and $C_e = 0$). The sole irreversibility in the cycle is heat resistance. The time of the two adiabatic processes is negligible (i.e. $\tau_a = \tau_b = 0$) compared to the time spent on the isomagnetic processes. The cycle period, power output and efficiency can be, respectively, expressed simply as:

$$\tau = \frac{1}{2a\hbar^2 e^{q\beta_h\omega_a} (e^{\beta_h\omega_a} + 1)} \times \ln \left[\frac{\tanh(\beta_h\omega_a/2) - \tanh(\beta_1\omega_a/2)}{\tanh(\beta_h\omega_a/2) - \tanh(\beta_3\omega_b/2)} \right] + \frac{1}{2a\hbar^2 e^{q\beta_c\omega_b} (e^{\beta_c\omega_b} + 1)} \times \ln \left[\frac{\tanh(\beta_c\omega_b/2) - \tanh(\beta_3\omega_b/2)}{\tanh(\beta_c\omega_b/2) - \tanh(\beta_1\omega_a/2)} \right] \quad (51)$$

$$P = \frac{1}{2}(\omega_a - \omega_b) \left[\tanh\left(\frac{\beta_1\omega_a}{2}\right) - \tanh\left(\frac{\beta_3\omega_b}{2}\right) \right] \tau^{-1} \quad (52)$$

$$\eta = 1 - \frac{\omega_b}{\omega_a}. \quad (53)$$

At high temperature limits, the cycle period and power output can be simplified to:

$$\tau = \frac{1}{4a\hbar^2} \ln \frac{\omega_a\omega_b(\beta_h - \beta_1)(\beta_c - \beta_3)}{(\omega_a\beta_h - \beta_3\omega_b)(\omega_b\beta_c - \beta_1\omega_a)}, \quad (54)$$

$$P = a\hbar^2(\omega_a - \omega_b)(\beta_1\omega_a - \beta_3\omega_b) \times \left[\ln \frac{\omega_a\omega_b(\beta_h - \beta_1)(\beta_c - \beta_3)}{(\omega_a\beta_h - \beta_3\omega_b)(\omega_b\beta_c - \beta_1\omega_a)} \right]^{-1}. \quad (55)$$

Case 2: Frictionless case (i.e. $\mu = 0$ and $C_e \neq 0$). The irreversibilities in the cycle are heat resistance and bypass heat leakage. Similar to the endoreversible case, by neglecting the time of the adiabatic processes (i.e. $\tau_a = \tau_b = 0$), one can simplify the efficiency as: Eq. (56) is given in Box III.

The cycle period and power output are independent of the bypass heat leakage, therefore, the cycle period and power output are still Eqs. (51) and (52), respectively. Based on Eqs. (52) and (56), one cannot derive the fundamental optimal relation analytically. Using numerical calculation, one obtains the $P/P_{\max, \mu=0, C_e=0} - \eta$ characteristic curve, as shown in Figure 4 (line 3), and the curve is monotonic increasing.

At high temperature limits, one can simplify Eq. (56) as: Eq. (57) is given in Box IV.

From Eqs. (55) and (57), one can derive the fundamental optimal relation, analytically, of the quantum Brayton heat engine in a frictionless case as:

$$P = C_e\alpha(\beta_c - \beta_h)(\omega_a - \omega_b) \frac{\eta}{\omega_a(1 - \eta) - \omega_b}. \quad (58)$$

Figure 5 (line 3) gives the $P/P_{\max, \mu=0, C_e=0} - \eta$ curve in the frictionless case and the curve is monotonic increasing.

Case 3: The case without bypass heat leakage (i.e. $\mu \neq 0$ and $C_e = 0$). The irreversibilities in the cycle are heat resistance and internal friction. In this case, one can simplify the efficiency as:

$$\eta = \left(1 - \frac{\omega_b}{\omega_a}\right) - \frac{\omega_b}{\omega_a} \left(\frac{1}{\tau_a} + \frac{1}{\tau_b}\right) \times \frac{2\mu^2}{\tanh(\beta_1\omega_a/2) - \tanh(\beta_3\omega_b/2) - 2\mu^2/\tau_a}. \quad (59)$$

The cycle period and power output are independent of bypass heat leakage, therefore, the cycle period and power output are still Eqs. (35) and (37), respectively. Based on Eqs. (37) and (59), one cannot derive the fundamental optimal relation analytically. Using numerical calculation, one obtains the $P/P_{\max, \mu=0, C_e=0} - \eta$ characteristic curve of the quantum heat engine without bypass heat leakage, as shown in Figure 4 (line 2), and the curve is parabolic-like.

At high temperature limits, one can simplify Eq. (59) as:

$$\eta = 1 - \frac{\omega_b}{\omega_a} - \frac{\omega_b}{\omega_a} \left(1 + \frac{\tau_a}{\tau_b}\right) \frac{4\mu^2}{(\tau_a\omega_a\beta_1 - \tau_a\omega_b\beta_3 - 4\mu^2)}. \quad (60)$$

Based on Eqs. (47) and (60), one cannot obtain the fundamental optimal relation of the quantum Brayton heat engine analytically. Using numerical calculations, one obtains the $P/P_{\max, \mu=0, C_e=0} - \eta$ characteristic curve, as shown in Figure 5 (line 2), and the $P/P_{\max, \mu=0, C_e=0} - \eta$ curve is parabolic-like.

8. Conclusions

For the irreversible quantum spin Brayton heat engine, the numerical examples show that both power output and

$$\eta = \frac{(\omega_a - \omega_b)[\tanh(\beta_1\omega_a/2) - \tanh(\beta_3\omega_b/2)]}{\omega_a[\tanh(\beta_1\omega_a/2) - \tanh(\beta_3\omega_b/2)] + 4C_e\hbar\omega_c e^{\lambda\hbar\beta_h\omega_c} [1 - (e^{\hbar\beta_h\omega_c} - 1)n_c]\tau}. \quad (56)$$

Box III:

$$\eta = \frac{a\hbar^2(\omega_a - \omega_b)(\beta_1\omega_a - \beta_3\omega_b)}{a\hbar^2\omega_a(\beta_1\omega_a - \beta_3\omega_b) + C_e\alpha(\beta_c - \beta_h) \ln \frac{\omega_a\omega_b(\beta_h - \beta_1)(\beta_c - \beta_3)}{(\omega_a\beta_h - \beta_3\omega_b)(\omega_b\beta_c - \beta_1\omega_a)}}. \quad (57)$$

Box IV:

efficiency have maxima. The power output versus efficiency characteristic curve is a beeline, and the efficiency is constant in the endoreversible case. Internal friction makes the power output versus efficiency characteristic curve a parabolic-like line, while the bypass heat leakage makes it a monotonic increasing line. When both internal friction and bypass heat leakage exists, the curve becomes a loop-shaped line. At high temperature limit, the power output versus efficiency characteristics is similar to that in a general case, and there is only a quantitative difference between them. Comparisons of the power output versus efficiency characteristics between this spin quantum heat Brayton engine, a Brayton heat engine working with classical working medium and a spin quantum Carnot heat engine, are made.

The obtained results are general; they can enrich the FTT theory for quantum thermodynamic cycles and can provide some guidelines for the optimal design of a real quantum heat engine.

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